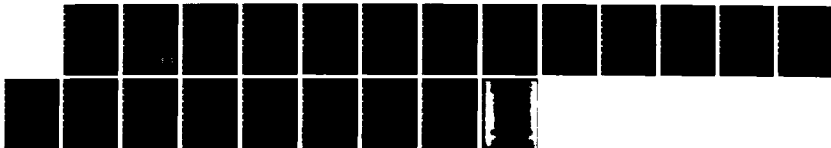
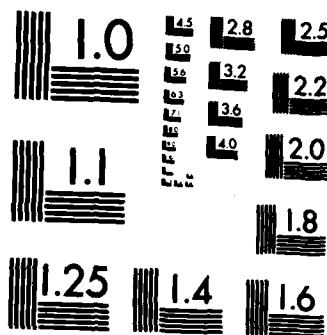


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FUEL EFFECTS ON SOOT FORMATION IN TURBOJET ENGINES

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4 May 1984

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<p>The sooting tendencies of sixteen Navy jet fuels and eight fuel blending components have been studied in laboratory flames to compare with results obtained in other programs using these fuels in turbojet engines and combustors. The average molecular weight, density, ASTM smoke point, and diffusion flame and premixed flame threshold sooting index of each fuel have been measured. An apparatus has been assembled to measure premixed flame soot yields using a multi-wavelength laser extinction technique. Experiments have also been performed on a six-component test fuel blended using pure hydrocarbon components. The diffusion</p>		

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flame soot threshold of this fuel can be predicted using the pure component values but the predicted premixed flame soot threshold is larger than measured. Experiments are planned to measure soot yields of the jet fuels and to correlate the laboratory measurements with engine test results.

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FOREWORD AND ACKNOWLEDGMENTS

This is the first technical progress report on work performed for the Naval Research Laboratory under Contract N00014-83-C-2311, which was initiated on 15 September 1983. The technical monitor at NRL is Dr. R.N. Hazlett. We gratefully acknowledge contributions to this effort by Dr. Sasha Madronich at AeroChem and helpful technical discussions with G. Speck and C.J. Nowack at NAPC in Trenton, NJ.

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I. INTRODUCTION

The ultimate objective of this program is to determine laboratory means of predicting the effects of fuel properties on smoke formation in turbojet engines. Specifically, ten fuel blends which are being evaluated in several combustors and engines in a Naval Air Propulsion Center (NAPC) fuel effects program are being studied in this work using laboratory flames, and the laboratory results and fuel analyses are being correlated with the combustor and engine results. To achieve this objective, we are measuring sooting tendencies of the test fuels, denoted NAPC 1-10, as well as several of the blending components which were used to make up the test fuels. Other laboratory experiments are being performed to elucidate how to calculate the properties of fuel mixtures from the properties of their pure components when these components are identified via chemical analyses.

II. PROGRESS

A. DIFFUSION FLAME SOOTING TENDENCIES

Twenty-four fuel samples were obtained from NAPC for use in this program. These fuels included fuels NAPC 1-10, NAPC 16-20, 22, and eight blending stocks. Several other blending stocks were no longer available, including the HCGO (hydrocracked gas oil) NAPC No. 148-81, used in NAPC-7, the DFM (diesel fuel marine) NAPC No. 118-81, used in NAPC-8, and Suntech furnace oil blend stock II, NAPC No. 139-81. Table 1 lists the fuels that were obtained along with their NAPC fuel numbers, their NAPC PE identifiers (NAPC No.), their NRL identifiers (NRL No.), and a descriptive name of each fuel. Also listed in the table are the hydrogen content, total aromatic content, and smoke point of each fuel as measured by NAPC, NRL, or reported by their contractors. Numerous other fuel properties have also been measured which will not be repeated here.

To obtain diffusion flame threshold sooting indices, TSI, as defined by Calcote and Manos,¹ we required measurements of the smoke point, density, and average molecular weight for each fuel. The ASTM smoke points were measured

1. Calcote, H.F. and Manos, D.M., "Effect of Molecular Structure on Incipient Soot Formation," *Combust. Flame* 49, 289 (1983).

TABLE 1. NAVY JET FUEL DATA

NAPC No.	Description	NAPC/NRL				
		NAPC PE No.	NRL No.	H%	Total Aromatic % (vol.)	SP
1	SUNTECH-1	140-81	81-13	13.36	32.14	17
2	SUNTECH-2	146-81	81-14	13.48	25.00	18
3	SUNTECH-3	147-81	81-15	13.66	23.63	20
4	SUNTECH-4	123-81	81-16	13.82	20.47	21
5	Low Aromatic JP-5	101-81	81-9	13.79	14.99	21
6	Fuel Oil #2	113-81	81-10	13.22	18.6	17
7	20/80 HCGO/NAPC-9	152-81	81-17	12.83	32.57	14
8	50/50 DFM/NAPC-5	119-81	81-12	13.54	21.0	16
9	HiAromatic JP-5	131-81	81-19	13.49	22.67	21
10	Oil Shale JP-5	106-81	J-22	13.70	24.0	21
16	JP-7	31-83	83-41	14.5	2.4 ^a	
17	DFM	30-83	83-42	13.20	20.1 ^a	17
18	Fuel Oil #2	32-83	84-3	13.4	23.7 ^a	
19	SUNTECH-A	49-83	83-43	12.2	32.9 ^a	
20	SUNTECH-B	54-83	83-44	12.9	27.1 ^a	
22	JP-5	44-83	83-45	13.7	17.6 ^a	
--	SUNTECH Kerosene	128-81	81-20	14.01	19.1 ^a	
--	SUNTECH Xylene Tower Bottoms	125-81	81-21	9.95	99.0 ^a	
--	SUNTECH Furnace Oil	127-81	81-22	13.96	15.4 ^a	
--	SUNTECH 40 Golden	129-81	81-24	12.74	26.4 ^a	
--	SUNTECH 60 Golden	130-81	81-25	12.48	39.1 ^a	
--	SUNTECH Kerosene	39-83	84-8	13.86	19.8 ^a	
--	SUNTECH #2 dist. Fuel Oil	40-83	84-9	13.52	18.9 ^a	
--	SUNTECH Catalytic Gas Oil	41-83	84-10	9.95	63.4 ^a	

^a Weight percent.

using a standard commercial ASTM apparatus and procedure² with the addition of a cathetometer to measure the flame heights. Our particular smoke point apparatus was delivered with the flame height scale, located inside the chimney behind the flame, neither perpendicular to the flame axis nor zeroed correctly with respect to the burner. The zero offset was large, about 2 mm, which could cause significant errors, especially for small flame heights. Thus the cathetometer, an Ealing Model 11-5279, allowed flame heights, referenced to the burner lip, to be read with 0.01 mm resolution so that measurement uncertainties in the smoke points were due to difficulties in defining exactly when the flame had been adjusted to the smoke point and in identifying exactly the position of the tip of the flame. Each day, before experiments were performed, the apparatus was calibrated using the toluene/isooctane mixtures specified in the ASTM test method D1322-75. The correction factors were small, about 1%, in all cases. The smoke points were measured three times by one operator and the values averaged. Table 2 lists these results which can be compared with values provided by NAPC (reported to the nearest unit value) listed in Table 1. Although there are differences as large as 2.6 units (for NAPC-8), the ASTM recommended 95% confidence limit for laboratory to laboratory reproducibility is three units, so there are no indications that the fuel samples provided to us differ significantly from those used in other parts of the fuel effects testing program.

Since fuel densities were not available, these were measured using a 10 cm³ pycnometer and precision balance. The exact pycnometer volume was determined using distilled water and the known density of water at the test temperature. Fuel density measurements were made at temperatures between 18-20°C. The results are listed in Table 2.

A significant reason for using diffusion flame TSIs instead of simply inverse smoke points is that correction is made for the flame height effects of the amount of air required to burn a given amount of each different fuel. This effect has been discussed previously.^{1,3} A good approximate correction is made

2. "Standard Test Method for Smoke Point of Aviation Turbine Fuels," ANSI/ASTM D1322-75, Reapproved 1980.

3. Gill, R.J., Olson, D.B., and Calcote, H.F., "Correlations of Soot Formation in Turbojet Engines and in Laboratory Flames," ASME Paper No. 84-GT-108, to be presented at 29th International Gas Turbine Conference, Amsterdam, Holland, 4-7 June 1984.

TABLE 2. NAVY JET FUEL DATA

AeroChem								
NAPC No.	Description	SP	Density g cm ⁻³	MW g mol ⁻¹	TSI _{exp} ^a	φ _c	TSI _{pf} ^b	T _{φ_c} , K
1	SUNTECH-1	17.0	0.8293	179	33.5	1.67	72	1720
2	SUNTECH-2	18.7	0.8338	189	32.1	1.66	73	1730
3	SUNTECH-3	20.8	0.8173	167	25.2	1.66	73	1720
4	SUNTECH-4	22.2	0.8160	176	24.9	1.70	68	1705
5	Low Aromatic JP-5	23.3	0.8143	171	22.9	1.67	72	1720
6	Fuel Oil #2	17.0	0.8379	189	35.4	1.69	70	1730
7	20/80 HCGO/NAPC-9	13.0	0.8435	171	42.2	1.58	83	1755
8	50/50 DFM/NAPC-5	18.6	0.8280	177	30.1	1.69	70	1710
9	HiAromatic JP-5	18.6	0.8203	161	27.3	1.68	71	1735
10	Oil Shale JP-5	20.6	0.8047	159	24.2	1.67	72	1700
16	JP-7	36.0	0.7980	171	14.3			
17	DFM	18.5	0.8318	196	33.7	1.66	73	1730
18	Fuel Oil #2	17.1	0.8373	195	36.4			
19	SUNTECH-A	10.4	0.8600	166	51.5	1.65	74	1785
20	SUNTECH-B	14.1	0.8416	168	38.1	1.63	77	1775
22	JP-5	20.8	0.8184	163	24.5			
--	SUNTECH Kerosene	22.9	0.8056	161	21.9	1.70	68	1700
--	SUNTECH Xylene Tower Bottoms	7.7	0.8760	118	49.4	1.57	84	1820
--	SUNTECH Furnace Oil	23.2	0.8138	188	25.4	1.70	68	1695
--	SUNTECH 40 Golden	12.5	0.8873	193	49.8	1.66	73	1745
--	SUNTECH 60 Golden	10.7	0.9028	233	70.8			
--	SUNTECH Kerosene	23.3	0.8025	159	21.1	1.65	74	1710
--	SUNTECH #2 dist. Fuel Oil	19.7	0.8308	193	31.1			
--	SUNTECH Catalytic Gas Oil	6.6	0.9427	177	87.6	1.53	88	1795

$$^a \text{TSI}_{\text{exp}} = -1.47 + 3.32 \left(\frac{\text{MW}}{\text{SP}} \right)$$

$$^b \text{TSI}_{\text{pf}} = 269 - 118 \phi_c$$

in calculating diffusion flame TSIs using the fuel average molecular weight. Experimental average molecular weights, MW, were not initially available for the fuels under test. In previous work^{3,4} where fuel samples were not available, we estimated MWs from the reported fractional distillation data on fuel blends using the assumption that the fuel mixtures were similar in boiling point vs. MW to the n-alkane series. This, of course, is a gross assumption, and so in the present program MWs were experimentally measured, using a benzene freezing point depression technique.⁵ Typically, an accurately known volume of about 1 cm³ of test fuel was mixed with 25 cm³ of reagent grade, dried benzene (with an experimental and literature freezing point of 5.51°C) and the freezing curve (temperature vs. time of the mixture) measured. A partial immersion precision calorimeter thermometer (Brooklyn Thermometer Co., Inc.), range = -1 to 11°C in 0.01°C divisions, was used to measure the temperatures as the mixture was cooled in a stirred insulated ice/water bath. Supercooling of the mixture was always observed, as is shown in Fig. 1 for NAPC-6. After crystals nucleated in the mixture, the temperature quickly rose to a constant value which was used as the mixture freezing point. The nominal 4% jet fuel/benzene mixture gave freezing point depressions of the order of one degree, which made the thermometer resolution sufficient to calculate the jet fuel molecular weight to a precision of about $\pm 1.5 \text{ g mol}^{-1}$. The molecular weights of several pure hydrocarbons were measured to investigate the true accuracy of the measurements, which resulted in an estimate of the overall accuracy of this technique to be $\pm 3 \text{ g mol}^{-1}$.

Average molecular weights for all 24 test fuels and blending agents are listed in Table 2. These values range from a low of 118 g mol⁻¹ for the xylene tower bottoms to a high of 233 g mol⁻¹ for the Suntech 60 Golden. These molecular weights were used in calculating diffusion flame TSIs, converting mass or volume measurements to molar quantities, and for calculating the fuel/air equivalence ratios in premixed flame experiments.

Diffusion flame threshold sooting indices were calculated for each fuel using the measured smoke point, molecular weight, and the relationship¹

$$\text{TSI} = a + b (\text{MW/SP})$$

4. Gill, R.J., Olson, D.B., and Calcote, H.F., "Correlations of Soot Formation in Turbojet Engines and in Laboratory Flames," Final Report, AeroChem TP-431, ESL-TR-83-31, May 1983.

5. Shoemaker, D.P. and Garland, C.W., Experiments in Physical Chemistry, 2nd Ed. (McGraw-Hill Book Company, New York, 1967) p. 132.

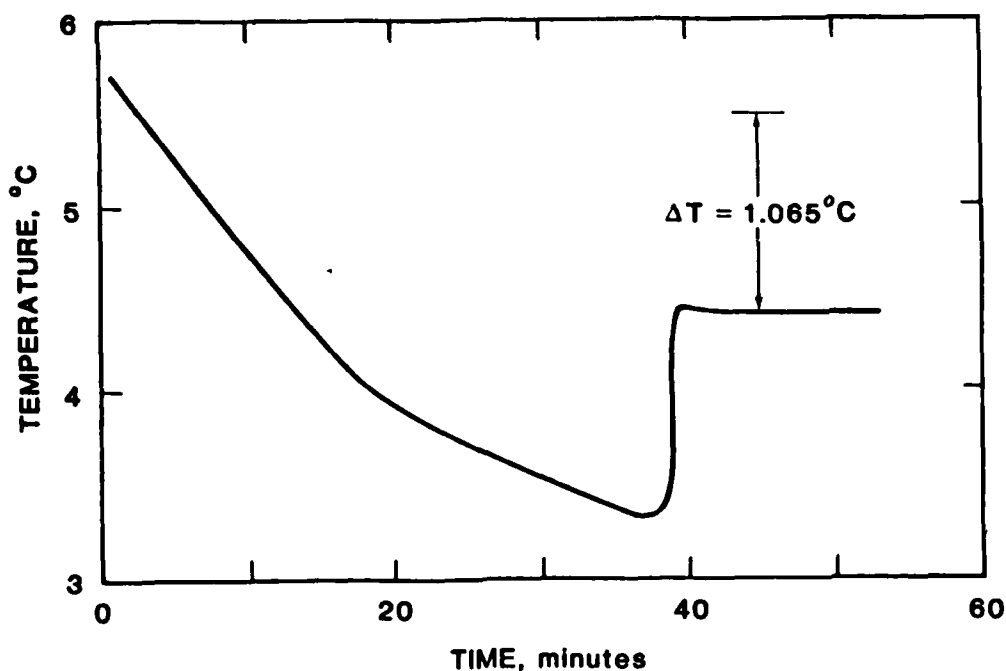


Figure 1. Freezing point depression curve for NAPC-6 in benzene from the observed difference in freezing points; the MW of NAPC-6 is calculated as 189 g mol^{-1} .

where the constants a and b correct for the effects of different experimental apparatuses, and are determined for each apparatus by measuring the smoke points of several previously studied pure hydrocarbons. Olson, Pickens, and Gill have recently reported an extensive list of diffusion flame TSIs⁶ which, when combined with other studies, results in a TSI data base for more than a hundred pure fuels. The calibration constants (a and b) for the ASTM apparatus were determined using eleven pure fuels, which gave the following equation which was used in this work

$$\text{TSI} = -1.47 + 3.32 (\text{MW/SP})$$

The threshold sooting indices so calculated are given in Table 2 where they are denoted as TSI_{exp} . The total range of TSIs for this set of fuels is from 14.3 to 87.6, but the values for NAPC 1-10 only cover the range from 22.9 to 42.2 with an average of 29.8 ± 6.1 .

The diffusion flame soot thresholds, i.e., TSIs, are therefore ready for correlation studies and comparison with values calculated using fuel analysis information.

6. Olson, D.B., Pickens, J.C., and Gill, R.J., "The Effects of Molecular Structure on Soot Formation. II. Soot Thresholds in Diffusion Flames," in preparation for Combust. Flame.

B. PREMIXED FLAME SOOTING TENDENCIES

Soot thresholds and flame temperatures have been measured in premixed flames of NAPC 1-10 and nine of the remaining 14 fuels and blending components. These experiments were performed using the burner and fuel vaporizer as shown in Fig. 2 which has been described previously.⁷ Briefly, the liquid fuels were metered using a syringe pump at about $1 \text{ cm}^3 \text{ min}^{-1}$ and spray vaporized using an air atomizing nozzle. Air was added to this mixture to achieve the desired final fuel/air ratio. A 2.2 cm diam multitubular stainless steel burner was used which had a fuel-rich shroud flame to reduce air entrainment and heat losses. The soot threshold is defined as the maximum fuel/air equivalence ratio, ϕ_c , at the first visual appearance of yellow thermal soot emission. Flame temperatures were measured using fine wire, 0.008 cm diam, Pt/Pt-10%Rh thermocouples (S type) and a calibrated Omega Model 199 digital temperature readout. These measurements were corrected for radiation and convection cooling effects with Kaskan's formula⁸ using an emissivity of 0.17 (clean pure platinum, total emissivity). Temperatures were measured as a function of equivalence ratio prior to the appearance of soot in the flame, and the temperature at ϕ_c extrapolated.

Soot threshold equivalence ratios and flame temperatures are shown in Table 2. The NAPC 1-10 fuels show similarities in these premixed flames, with a ϕ_c range of 1.58 to 1.71 and temperatures from 1700 to 1755 K. If NAPC-7 (20/80 mixture of HCGO and NAPC-9) is excluded, the ϕ_c range is only from 1.65 to 1.71 and the flame temperature range is only from 1700 to 1735 K, both of which are remarkably narrow ranges.

Premixed flame threshold sooting indices were calculated from the measured ϕ_c values using the TSI definition¹

$$\text{TSI}_{\text{pf}} = a' - b'(\phi_c)$$

where the calibration constants a' and b' are again characteristic of the experimental apparatus and are determined by measuring soot thresholds for several

-
7. Olson, D.B. and Pickens, J.C., "The Effects of Molecular Structure on Soot Formation. I. Soot Thresholds in Premixed Flames," *Combust. Flame*, in press.
 8. Kaskan, W.E., "The Dependence of Flame Temperature on Mass Burning Velocity," Sixth Symposium (International) on Combustion (Reinhold Publishing Corp., New York, 1957) p. 134.

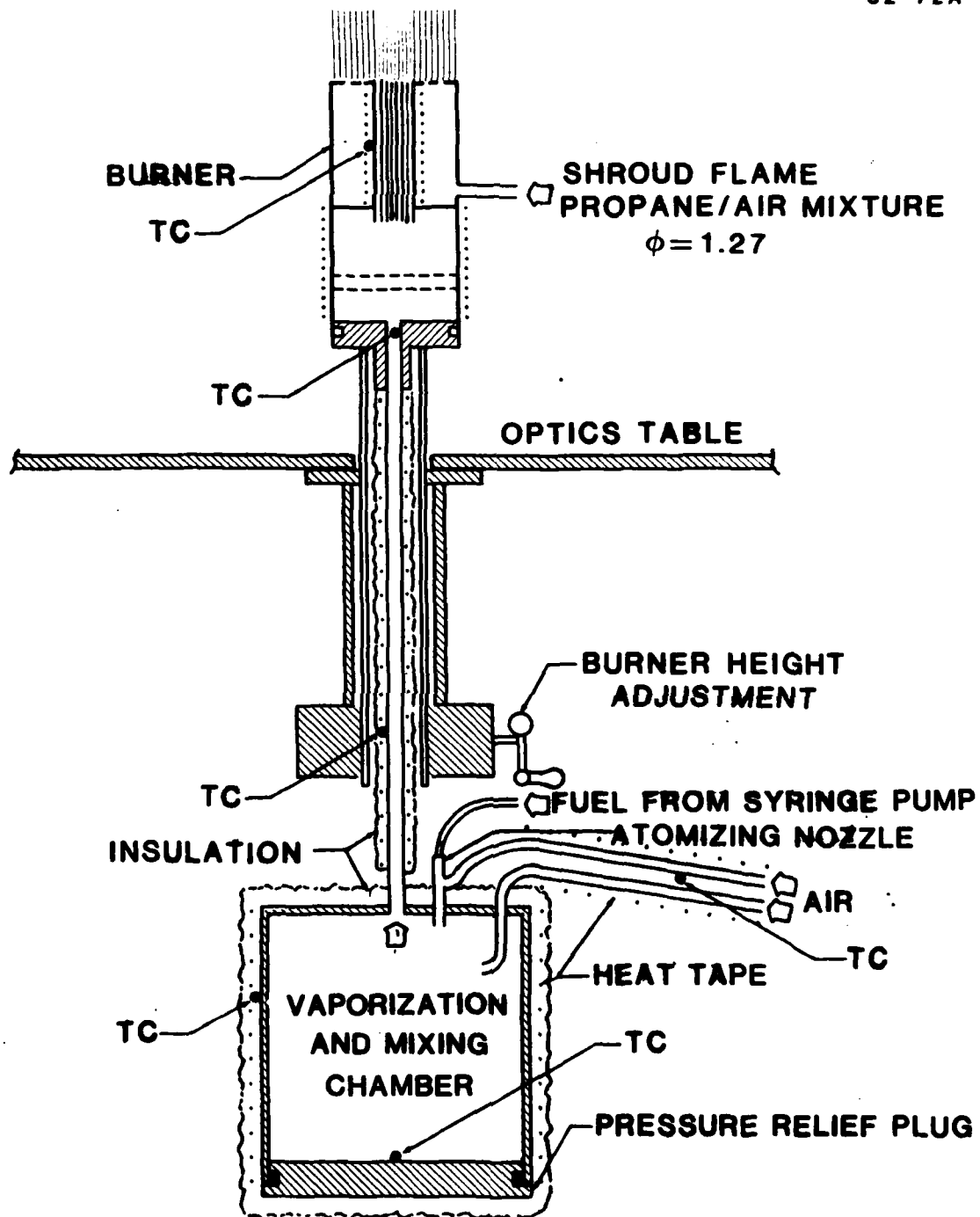


Figure 2. Premixed flame burner and fuel vaporizer.

previously studied pure fuels. The previous calibration of Olson and Pickens⁷ was confirmed to be accurate, so the final equation was

$$TSI_{pf} = 269 - 118 (\phi_c)$$

TSI_{pf} values so calculated are given in Table 2, and range from 67 to 83 for NAPC 1-10, or only from 67 to 74 without NAPC-7. Thus, if NAPC 1-10 show strong variations in smoke related performance in the engine tests, we would not anticipate that premixed flame TSIs would be a good correlating parameter of the test results.

TSI_{pf} and flame temperatures will be measured for the remaining fuels in future work.

C. PREMIXED FLAME SOOT YIELDS

In all practical applications, it is the quantity of soot produced at some fuel/air equivalence ratio beyond the soot threshold rather than the soot threshold itself that is probably most important. Since soot thresholds in premixed flames and smoke points in diffusion flames are the main parameters which have been previously studied, they have been used as initial correlation parameters. In this program we will also measure the premixed flame soot yields of NAPC 1-10 and the other fuels to investigate whether soot yields correlate the engine test results better than soot thresholds.

The apparatus for performing these measurements is shown in Fig. 3. Using the same burner and fuel vaporizer as used to measure soot thresholds, the soot volume fractions (total volume of soot particles per unit flame volume) will be measured using a multiwavelength laser extinction technique. The red He-Ne and blue or green tunable argon ion laser beams are modulated, passed through the flame several times using multipass reflection optics, and the decreased beam intensity, I , is measured vs. the original beam intensity, I_0 , at various heights above the burner and at several fuel/air ratios using a phase-locked amplifier. This technique has been used previously at AeroChem⁹ and elsewhere¹⁰ with good success. The procedures for calculating soot volume

9. Olson, D.B., "Soot Formation in Synfuels," Final Report, AeroChem TP-433, DOE/PC/30304-5, June 1983.

10. Pagni, P.J. and Bard, S., "Particulate Volume Fractions in Diffusion Flames," Seventeenth Symposium (International) on Combustion (The Combustion Institute, Pittsburgh, 1979) p. 1017.

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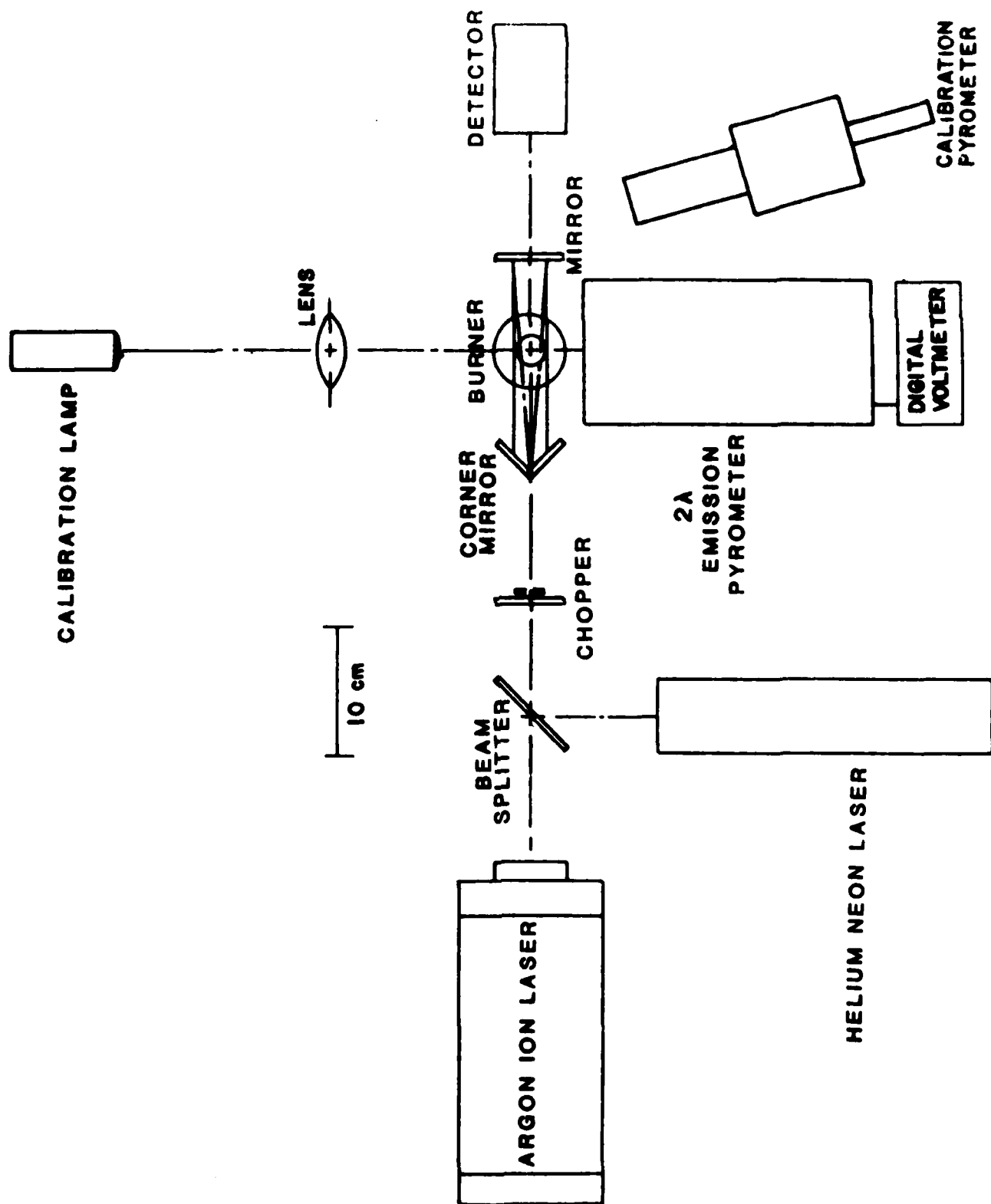


Figure 3. Laser extinction apparatus for measuring soot yields.

fractions, f_v , from the measured laser extinctions at several wavelengths utilizing Mie scattering theory, reasonable assumptions about the particle size distribution, and the soot optical properties as measured by Lee and Tien,¹¹ have been discussed in detail elsewhere.¹⁰

The apparatus has now been reassembled. Soot volume fractions were measured at several equivalence ratios for toluene/air flames to compare with results from our previous work⁹ to test out the apparatus. Excellent agreement was obtained so the apparatus and procedures are considered ready for routine measurements. These are currently underway.

Madronich¹² has analyzed the sooting tendencies of multicomponent mixtures compared to the pure fuel soot and mixture thresholds and yields observed by Olson and coworkers.^{6,7,9,13} By assuming that the soot production of each fuel component is independent of the presence of other components, except for the sharing of the available oxidizer, he was able to derive the previously observed mixture rule for premixed flames.

D. AEROCHEM TEST FUEL

In addition to performing the measurements discussed above on the NAPC test fuels and blending agents, which are being chemically analyzed in some detail, we have also used a six component fuel blended from pure hydrocarbons. The purpose of these measurements is to have data on a simpler fuel mixture of accurately known composition against which to test the MW measurement and proposed mixture rules for calculating fuel blend properties using known pure component properties. This fuel, denoted AeroChem-A, has the composition given in Table 3. From this known composition the hydrogen content is 13.53%, the total aromatic content is 22.71% (by weight), and the average molecular weight is 137.3 g mol⁻¹.

-
11. Lee, S.C. and Tien, C.L., "Optical Constants of Soot in Hydrocarbon Flames," Eighteenth Symposium (International) on Combustion (The Combustion Institute, Pittsburgh, 1981) p. 1159.
 12. Madronich, S., "Prediction of Fuel Mixture Soot Production in Premixed Flames," to be submitted to Combust. Sci. Tech.
 13. Gill, R.J. and Olson, D.B., "Estimation of Soot Thresholds for Fuel Mixtures," Combust. Sci. Tech., in press.

TABLE 3. COMPOSITION AND DIFFUSION FLAME TSI OF AEROCHEM-A

Component	Component MW	Mole Fraction	TSI _i	X _i • TSI _i
n-Heptane	100.2	0.267	2.6	0.7
n-Tetradecane	198.4	0.270	5.4	1.4
Decalin	138.3	0.187	15	2.8
Toluene	92.1	0.140	44	6.2
Tetralin	132.2	0.109	61	6.6
1-Methylnaphthalene	142.2	<u>0.027</u>	91	<u>2.5</u>
		1.000		20.2

Measurements on AeroChem-A yielded the following results:

MW	=	134.4 g mol ⁻¹
Density	=	0.7996 g mol ⁻¹
Smoke Point	=	23.5 ± 0.1
TSI _{exp}	=	17.9 based on the theoretical MW
φ _c	=	1.69
TSI _{pf}	=	69
T (φ _c)	=	1695 K

Thus the smoke point, premixed flame TSI, and flame temperature of AeroChem-A are similar to the NAPC test fuels. The MW and density are slightly lower. We note that the difference between the calculated and measured MW, 137.3 vs. 134.4 g mol⁻¹, is within the stated ± 3 g mol⁻¹ accuracy of the freezing point depression measurements.

Using the Gill and Olson diffusion flame mixture rule,¹³

$$TSI_{mix} = \sum_i X_i TSI_i$$

a calculation of the TSI of AeroChem-A from the measured TSIs of the six components was made. The individual component TSIs⁶ and the partial molar contribution of each component to the total are given in Table 3. The calculated value is larger than observed experimentally, 20.2 calculated vs. 17.9 measured, or about 10% difference. The corresponding calculated vs. measured smoke points are 21.1 vs. 23.5. This is not considered to be a particularly good comparison, but it is acceptable. Probably one or more of the component TSIs would be slightly different if measured on this particular apparatus; recall that these TSI_i values were taken from a review⁶ of all previous work which averaged data

from several different types of burners. This explanation of the error was checked for the TSI of toluene. The literature averaged value is $TSI = 44$, but in this work we measured $TSI = 39$ using the ASTM apparatus. This difference for toluene alone changes the calculated TSI_{mix} of AeroChem-A to 19.5, much closer to the measured value.

One insight provided by this calculation is the ability to identify which components in the fuel mixture dominate the soot threshold behavior. Looking at the column in Table 3 labeled " $X_i \cdot TSI_i$," we observe that the aromatic components essentially control the soot threshold since they contribute 76% of the TSI but comprise only 28 mole percent (or 22.7 weight percent) of the mixture. Also the decalin fraction can be identified as more important toward determining the soot threshold than both of the n-alkanes combined, even though there is almost three times as much of the n-alkanes.

A similar calculation was performed for AeroChem-A using the premixed flame mixture rule¹³

$$(1.1) \quad TSI_{mix} = \sum_i X_i (1.1) TSI_i$$

This gave a calculated TSI of 82 vs. a measured value of 69. This large discrepancy is unexplained at this time.

III. SUMMARY AND PLANS

A large fraction of the planned laboratory work has been completed. All of the diffusion flame TSIs, premixed flame TSIs, and flame temperatures for NAPC 1-10, and for all but three of the blending agents have been measured. The main remaining laboratory effort is to measure soot volume fractions, i.e., soot yields, from premixed flames of the various fuels. This work is currently underway.

Correlations of the fuel parameters measured in this and other work with engine test results will be performed for the T56 and TF30 combustor rigs,¹⁴⁻¹⁶ the only NAPC data available at this time, in the near future.

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